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Published in:
Proceedings - ECCOMAS Multibody Dynamics 2013

Publication date:
2013

Document Version
Publisher's PDF, also known as Version of record

ECCOMAS Multibody Dynamics 2013
1-4 July, 2013, University of Zagreb, Croatia

Multibody motion in implicitly constrained director format with links via explicit constraints

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Abstract

A conservative time integration algorithm is developed for constrained mechanical systems of kinematically linked rigid bodies based on convected base vectors. The base vectors are represented in terms of their absolute coordinates, hence the formulation makes use of three translation components, plus nine base vector components for each rigid body. Both internal and external constraints are considered. Internal constraints are used to enforce orthonormality of the three base vectors by constraining the equivalent Green strain components, while the external constraints are associated with the presence of kinematic joints for linking bodies together. The equations of motion are derived from Hamilton's equations with an augmented Hamiltonian in which internal and external constraints initially are included via Lagrange multipliers. Subsequently the Lagrange multipliers associated with internal constraints are eliminated by use of a set of displacement-momentum orthogonality conditions, leaving a set of differential equations in which additional algebraic constraints are needed only for imposing external constraints. The equations of motion are recast into a conservative mean-value and finite difference format based on the finite increment of the Hamiltonian. Examples dealing with a hanging chain represented by a four body linkage serve to demonstrate the efficiency and accuracy of the algorithm.

Keywords: *multibody dynamics, implicit constraints, conservative time integration*

1 Introduction

Integration of finite rotations plays a major role in dynamic analysis of multibody systems. In particular, conservative integration schemes have been the scope of extensive research during the last two decades. These are based on an integrated form of the equations of motion, and thus they can be designed to obey major conservation laws such as conservation of energy and momentum by a proper discretization, often in terms of a combination of mean values and increments. The basic idea is illustrated in [1] for rigid body dynamics and extended to non-linear elastic models by introducing the concept of finite derivatives in [2]. Furthermore application to constrained multibody systems is presented in [3].

While numerical procedures for translations are fairly well established, special parameterizations accounting for the fact that finite rotations do not combine in the form of incremental vector addition have to be used. A common way is to represent rotations in terms of four quaternion parameters supplemented by a normalization constraint. In [4] the constraint is enforced via a Lagrange multiplier, while it is demonstrated in [5] that the constraints are embedded implicitly in the evolution equations, when a projection operator is introduced on the external potential gradient. Alternatively, the kinematics can be formulated directly in terms of the time derivatives of the director components with holonomic constraints, [6]. This leads to a very simple formulation, but at the expense of a considerable increase of the original 3 translation and 3 rotation variables to 3 translations, 3×3 director components, plus 6 or even 12 Lagrange multipliers for enforcing the constraints.

In the present paper the kinematics of the rigid body is formulated in terms of the instantaneous angular velocity, which takes a particularly simple form when expressed in terms of directors, [7]. This approach has the advantage that the incremental form of the internal director constraints can be embedded in the equations of motion by generalizing the concept of implicit constraints introduced in connection with quaternion parameters in [5], and thus the explicit use of Lagrange multipliers is limited to the external constraints associated with connecting multiple bodies.

The equations of motion are derived from an augmented Hamiltonian where internal and external constraints initially are included via Lagrange multipliers. However, the special form of the inertial tensor based on director components serves to identify six orthogonality conditions between the director components and their conjugate momentum vector, which can be used to eliminate the Lagrange multipliers associated with the internal constraints. This leads to a modification of the dynamic equation where the effect of internal constraints is represented by a projection operator acting on the unconstrained potential and external constraint gradients.

The equivalent discretized system of equations follow by forming a finite increment of the Hamiltonian. This procedure defines a proper choice of increments and mean values leading to an algorithm with energy and momentum conserving properties. In particular, constraints are introduced in incremental form, whereby the Lagrange multipliers serves the role as effective reaction forces needed to uphold the constraints over the interval. The accuracy and conservative properties of the presented algorithm are illustrated in terms of a hanging chain formed by four kinematically linked rigid bodies.

2 Convected base vector representation

Let the orientation of a rigid body be expressed in terms of an orthonormal director frame $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$ centered at a point O defined by the position vector $\mathbf{q}_0$. The global components $\mathbf{x}$ of a point located inside the rigid body with local coordinates $\mathbf{x}_0$ can then be expressed as

$$\mathbf{x}(t) = \mathbf{q}_0(t) + \mathbf{Q}(t)\mathbf{x}_0, \tag{1}$$

in terms of the deformation gradient tensor $\mathbf{Q}$, defined by

$$\mathbf{Q} = [\,\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\,] = \frac{\partial \mathbf{x}}{\partial \mathbf{x}_0}. \tag{2}$$

The global components of the vector $\mathbf{q} = [\mathbf{q}_0^T, \mathbf{q}_1^T, \mathbf{q}_2^T, \mathbf{q}_3^T]^T$ constitute the independent variables of the present formulation. The base vector components are conveniently collected in the vector $\boldsymbol{q} = [\mathbf{q}_1^T, \mathbf{q}_2^T, \mathbf{q}_3^T]^T$. In order to represent a proper rigid body rotation, the base vectors $\boldsymbol{q}_j$ must remain as an orthonormal triple, as expressed by the kinematic constraints

$$\mathbf{e} = \frac{1}{2}\begin{bmatrix} \mathbf{q}_1^T\mathbf{q}_1 - 1 \\ \mathbf{q}_2^T\mathbf{q}_2 - 1 \\ \mathbf{q}_3^T\mathbf{q}_3 - 1 \\ \mathbf{q}_2^T\mathbf{q}_3 + \mathbf{q}_3^T\mathbf{q}_2 \\ \mathbf{q}_3^T\mathbf{q}_1 + \mathbf{q}_1^T\mathbf{q}_3 \\ \mathbf{q}_1^T\mathbf{q}_2 + \mathbf{q}_2^T\mathbf{q}_1 \end{bmatrix} = \mathbf{0}. \tag{3}$$

In principle, this quadratic set of constraints is equivalent to vanishing of all Green strain components. In the present formulation the kinematic constraints appear via their time derivatives in the form

$$\dot{\mathbf{e}} = \mathbf{C}(\mathbf{q})\,\dot{\mathbf{q}} = \mathbf{C}(\dot{\mathbf{q}})\,\mathbf{q} = \mathbf{0}\,, \tag{4}$$

where $\mathbf{C}(\mathbf{q})$ is the gradient matrix associated with the constraints (3), given by

$$\mathbf{C}(\mathbf{q}) = \frac{\partial \mathbf{e}}{\partial \mathbf{q}} = \begin{bmatrix} \mathbf{0} & \mathbf{q}_1^T & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{q}_2^T & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{q}_3^T \\ \mathbf{0} & \mathbf{0} & \mathbf{q}_3^T & \mathbf{q}_2^T \\ \mathbf{0} & \mathbf{q}_3^T & \mathbf{0} & \mathbf{q}_1^T \\ \mathbf{0} & \mathbf{q}_2^T & \mathbf{q}_1^T & \mathbf{0} \end{bmatrix}. \tag{5}$$

By selecting the origin O of the convected base vectors such that it coincides with the center of mass, the kinetic energy takes a particularly simple form where the contributions from translational and rotational motion decouple. The kinetic energy of rigid body can then be expressed in terms of the linear velocity $\mathbf{v}$ and global components of local angular velocity $\boldsymbol{\Omega}$, as

$$T = \tfrac{1}{2}M\,\mathbf{v}^T\mathbf{v} + \tfrac{1}{2}\boldsymbol{\Omega}^T\boldsymbol{J}\,\boldsymbol{\Omega}\,, \tag{6}$$

where M and $\mathbf{J}$ are the mass and the constant inertia tensor, respectively.

The translational velocities $\mathbf{v}$ follow directly by time differentiation of the position vector components $\mathbf{q}_0$, while the local components of the angular velocities in terms of base vectors can be obtained by projection of the derivative $\dot{\boldsymbol{q}}_i$ on the vectors $\boldsymbol{q}_j$. This can be expressed in the compact matrix form

$$\begin{bmatrix} \mathbf{v} \\ \boldsymbol{\Omega} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\frac{1}{2}\boldsymbol{G}(\boldsymbol{q}) \end{bmatrix} \begin{bmatrix} \dot{\mathbf{q}}_0 \\ \dot{\boldsymbol{q}} \end{bmatrix} = \mathbf{G}(\mathbf{q})\,\dot{\mathbf{q}}\,, \tag{7}$$

in terms of the 3×9 matrix

$$G(q) \;=\; \begin{bmatrix} \mathbf{0} & -\mathbf{q}_3^T & \mathbf{q}_2^T \\ \mathbf{q}_3^T & \mathbf{0} & -\mathbf{q}_1^T \\ -\mathbf{q}_2^T & \mathbf{q}_1^T & \mathbf{0} \end{bmatrix} . \tag{8}$$

The $\mathbf{G}$-matrix has the same structure in terms of the base vectors $\boldsymbol{q}$ as the skew symmetric matrix associated with the vector product, hence the very structure implies orthogonality with respect to $\boldsymbol{q}$. It is an important property that the columns of the matrix $\mathbf{G}(\mathbf{q})$ spans the null-space of the constraint matrix $\mathbf{C}(\mathbf{q})$ when $\boldsymbol{q}$ constitutes an orthonormal base. This can be expressed by the orthogonality condition

$$\mathbf{C}(\mathbf{q})\,\mathbf{G}(\mathbf{q})^T \;=\; \mathbf{0}\,. \tag{9}$$

In the particular case when the vectors $\boldsymbol{q}_j$ are orthonormal, the matrix furthermore satisfies the relation

$$\mathbf{G}(\mathbf{q})\,\mathbf{G}(\mathbf{q})^T \;=\; \begin{bmatrix} \mathbf{I} & \\ & \frac{1}{2}\mathbf{I} \end{bmatrix} , \tag{10}$$

which serves to identify a generalized inverse of the matrix $\mathbf{G}(\mathbf{q})$.

Upon substitution of the velocity, expressed in terms of the independent coordinates via (7) into (6), the kinetic energy for a rigid body takes the form

$$T \;=\; \tfrac{1}{2}\left[\begin{array}{cc} \mathbf{v} & \boldsymbol{\Omega} \end{array}\right] \begin{bmatrix} M\mathbf{I} & \\ & \boldsymbol{J} \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ \boldsymbol{\Omega} \end{bmatrix} \;=\; \tfrac{1}{2}\dot{\mathbf{q}}^T\mathbf{G}(\mathbf{q})^T\mathbf{J}\,\mathbf{G}(\mathbf{q})\,\dot{\mathbf{q}}\,, \tag{11}$$

where the inertia tensor $\mathbf{J}$ is introduced as a block diagonal form of the mass M and the local components of the moment of inertia tensor $\boldsymbol{J}$. The relation (11) thereby represents the kinetic energy for rigid body motion when the base vector components $\boldsymbol{q}_j$ satisfy the constraints (3).

3 Constrained rigid body motion

The equations describing constrained motion of a rigid body are derived via Hamilton's equations based on a set of generalized displacements, here expressed in terms of the vector components $\mathbf{q}$, and their conjugate momentum variables $\mathbf{p}$. This leads to a set of first order evolution equations for $\dot{\mathbf{q}}$ and $\dot{\mathbf{p}}$, see e.g. [8].

3.1 Hamilton's equations

The generalized momentum vector $\mathbf{p} = [\mathbf{p}_0^T, \mathbf{p}_1^T, \mathbf{p}_2^T, \mathbf{p}_3^T]^T$ associated with the generalized coordinates $\mathbf{q}$, follow by differentiation of the kinetic energy (11) with respect to the generalized velocity $\dot{\mathbf{q}}$, as

$$\mathbf{p} \;=\; \frac{\partial T}{\partial \dot{\mathbf{q}}^T} \;=\; \mathbf{G}(\mathbf{q})^T\mathbf{J}\,\mathbf{G}(\mathbf{q})\,\dot{\mathbf{q}}\,. \tag{12}$$

Since Hamilton's equations are based on the generalized coordinates $\mathbf{q}$ and their conjugate momentum components $\mathbf{p}$ it is convenient to use this relation to eliminate the velocity $\dot{\mathbf{q}}$ from the kinetic energy (11). This task can be performed by use of the inverse relation of (12), which is easily obtained by pre-multiplication with $\mathbf{G}(\mathbf{q})$. For a rigid body the base vectors $\boldsymbol{q}_j$ are orthonormal, hence use of the orthogonality relation (10) leads to the following relation for the kinetic energy

$$T(\mathbf{q},\mathbf{p}) \;=\; \tfrac{1}{2}\mathbf{p}^T\mathbf{G}(\mathbf{q})^T \begin{bmatrix} M^{-1}\mathbf{I} & \mathbf{0} \\ \mathbf{0} & 4\boldsymbol{J}^{-1} \end{bmatrix} \mathbf{G}(\mathbf{q})\,\mathbf{p} \;=\; \tfrac{1}{2}\mathbf{p}^T\mathbf{G}(\mathbf{q})^T\mathbb{J}^{-1}\mathbf{G}(\mathbf{q})\,\mathbf{p}\,. \tag{13}$$

Here, the effect of the factor $\frac{1}{2}$ in the lower block matrix of (10) has been embedded in the inverse inertia tensor $\mathbb{J}^{-1}$ by multiplication of the lower 3 by 3 block matrix representing the inertia tensor $\boldsymbol{J}^{-1}$ by a factor 4.

The present formulation for constrained rigid body motion makes use of an augmented form of Hamiltonian's energy functional where the sum of the kinetic energy $T(\mathbf{q},\mathbf{p})$ from (13) and potential energy function $V(\mathbf{q})$ is supplemented by a set of internal constrains in the form (3), and external constraints $\boldsymbol{\Phi}(\mathbf{q})$ associated with the presence of kinematic joints. The augmented Hamiltonian hereby takes the form

$$H(\mathbf{q},\mathbf{p},\gamma,\boldsymbol{\lambda}) \;=\; T(\mathbf{q},\mathbf{p}) \;+\; V(\mathbf{q}) \;+\; \boldsymbol{\Phi}(\mathbf{q})^T\boldsymbol{\lambda} \;-\; \mathbf{e}(\mathbf{q})^T\boldsymbol{\gamma}\,. \tag{14}$$

The external constraints enter via a vector of Lagrange multipliers $\boldsymbol{\lambda}$. Similarly, the zero strain constraints $\mathbf{e}(\mathbf{q})$ from (3) are initially introduced via the six component vector of Lagrange multipliers γ. However, a particular feature of the present formulation is these can be eliminated by using a displacement-momentum orthogonality relation.

The equations of motion now follow by differentiation of the extended Hamiltonian (14) with the kinetic energy expressed by (13) in terms of **q** and **p**, whereby

$$\dot{\mathbf{q}} \;=\; \frac{\partial H}{\partial \mathbf{p}^T} \;=\; \mathbf{G}(\mathbf{q})^T \mathbb{J}^{-1} \mathbf{G}(\mathbf{q})\,\mathbf{p}\,, \tag{15}$$

$$\dot{\mathbf{p}} \;=\; -\frac{\partial H}{\partial \mathbf{q}^T} \;=\; -\,\mathbf{G}(\mathbf{p})^T \mathbb{J}_0^{-1} \mathbf{G}(\mathbf{p})\,\mathbf{q} \,-\, \frac{\partial V}{\partial \mathbf{q}^T} \,-\, \Big(\frac{\partial \boldsymbol{\Phi}}{\partial \mathbf{q}^T}\Big)^T \boldsymbol{\lambda} \,+\, \mathbf{C}(\mathbf{q})^T \gamma\,. \tag{16}$$

Here, the matrix $\mathbb{J}_0^{-1} = \mathrm{diag}[\mathbf{0},\, 4\mathbf{J}^{-1}]$ is introduced in the dynamic equation (16) since the translational kinetic energy only depends on the momentum components $\mathbf{p}_0$. Furthermore, the matrix $\mathbf{C}(\mathbf{q})^T$ is the derivative of the internal constraint relation with respect to **q** as expressed by (4). For a constrained mechanical system the kinematic equation (15) and dynamic equation (16) must be supplemented by additional algebraic constraint equations. For the external constraints, these follow by differentiation with respect to $\boldsymbol{\lambda}$, as

$$\frac{\partial H}{\partial \boldsymbol{\lambda}^T} \;=\; \boldsymbol{\Phi}(\mathbf{q}) = \mathbf{0}\,. \tag{17}$$

Similarly the constraint equations associated with internal constraint could be obtained by differentiation with respect to γ. However, as illustrated in the following section the Lagrange multipliers γ associated with internal constraints can be eliminated, hence no additional equations are required.

3.2 Elimination of internal constraints

A key point in the present formulation is the elimination of the Lagrange multipliers γ, which can be performed by using a set of orthogonality relations between **q** and **p**, [7]. These can be established by pre-multiplication of the relation (12) defining the momentum components **p** with the constraint matrix $\mathbf{C}(\mathbf{q})$. This leads to the following relation

$$\mathbf{C}(\mathbf{q})\,\mathbf{p} \;=\; \mathbf{0}\,, \tag{18}$$

when the relation (9), valid for orthogonal base vectors **q**, is accounted for. It is important to notice that the displacement-momentum orthogonality condition (18) constitutes an independent complement to the kinematic relation (4), rather than a simple reformulation, and serves the basis for eliminating the Lagrange multipliers. The actual elimination process is performed via the time derivative of (18), given by

$$\mathbf{C}(\mathbf{p})\,\dot{\mathbf{q}} \,+\, \mathbf{C}(\mathbf{q})\,\dot{\mathbf{p}} \;=\; \mathbf{0}\,. \tag{19}$$

By substitution of the derivatives from (15) and (16) an explicit equation for the Lagrange multipliers γ can be established. The structure of $\mathbf{C}(\mathbf{q})$ eliminates contributions from translational components. Furthermore, the contributions from the first terms in (15) and (16) cancel since the roles of **q** and **p** can be interchanged due to the structure of the lower block $\boldsymbol{G}(\boldsymbol{q})$ in (8) associated with rotational components, whereby the Lagrange multipliers γ can be determined as

$$\gamma \;=\; \big[\mathbf{C}(\mathbf{q})\,\mathbf{C}(\mathbf{q})^T\big]^{-1}\mathbf{C}(\mathbf{q})\Big[\frac{\partial V}{\partial \mathbf{q}^T} \,+\, \Big(\frac{\partial \boldsymbol{\Phi}}{\partial \mathbf{q}}\Big)^T \boldsymbol{\lambda}\Big]\,. \tag{20}$$

It is noticed that the Lagrange multipliers associated with internal constraints vanish in the absence of external loads and external constraints, which implies that the homogenous equations could be solved directly without explicit imposing internal constraints. When the Lagrange multiplier vector γ expressed by (20) is inserted back into (16), the modified dynamic equation takes the form,

$$\begin{aligned}\dot{\mathbf{p}} \;=\; &-\,\mathbf{G}(\mathbf{p})^T \mathbb{J}^{-1} \mathbf{G}(\mathbf{p})\,\mathbf{q} \\ &-\,\Big(\mathbf{I} \,-\, \mathbf{C}(\mathbf{q})^T\big[\mathbf{C}(\mathbf{q})\,\mathbf{C}(\mathbf{q})^T\big]^{-1}\mathbf{C}(\mathbf{q})\Big)\Big[\frac{\partial V}{\partial \mathbf{q}^T} \,+\, \Big(\frac{\partial \boldsymbol{\Phi}}{\partial \mathbf{q}}\Big)^T \boldsymbol{\lambda}\Big]\,.\end{aligned} \tag{21}$$

It is seen that the effect of eliminating the Lagrange multipliers via the orthogonality relation (18) is equivalent to introduction of a projection operator in front of the gradients of the external potential and the external constraints, which eliminates their projection on the deformation modes from the unconstrained gradients.

4 Conservative time integration

In essence, conservative integration amounts to ensuring that the discrete form of the equations of motion reproduces the correct incremental change of energy and momentum over a finite time increment. This is different from collocation based methods where the typical procedure is to solve the equations of motion at discrete points in time via truncated series expansions. Similarly, when it comes to enforcements of constraints in conservative schemes via Lagrange multipliers, the role of the multipliers is to ensure that the work performed by constraints over the interval vanishes. Hence rather than enforcing constraints explicitly at the interval boundaries, the Lagrange multipliers can be interpreted as interval bounded quantities ensuring that the incremental change vanishes. By initiating a numerical integration from a state that satisfy constraints, the correct representation of the incremental form over each interval, will ensure satisfaction of the constraints at any later stages within the iteration tolerance.

A conservative discretization of the equations of motion (15) and (16) follows directly by equating the finite increment of the Hamiltonian (14) to zero. This can be expressed in the form

$$\Delta H(\mathbf{q},\mathbf{p},\boldsymbol{\lambda}) \,=\, \Delta\mathbf{q}^T\frac{\partial H_*}{\partial\mathbf{q}^T} \,+\, \Delta\mathbf{p}^T\frac{\partial H_*}{\partial\mathbf{p}^T} \,+\, \Delta\boldsymbol{\lambda}^T\frac{\partial H_*}{\partial\boldsymbol{\lambda}^T} \,=\, 0\,, \tag{22}$$

where the asterisk denotes discrete derivatives of H, which combined with the increments $\Delta\mathbf{q}$ and $\Delta\mathbf{p}$, lead to the correct finite increment of the Hamiltonian. The individual terms follow by taking the increment of (14). The kinetic energy (13) is a bi-quadratic form in $\mathbf{q}$ and $\mathbf{p}$, hence its increment can be expressed as twice the product of the first factor and the mean of the second factor. The external potential $V(\mathbf{q})$ and the external constraints $\boldsymbol{\Phi}(\mathbf{q})$ are introduced via their finite derivatives, [2], while the discrete form of the internal constraints (3) can be expressed explicitly by a combination of increments and mean values due to its homogeneous quadratic form. The Lagrange multipliers are represented by constants over each interval and serves the role as the effective reaction forces needed for upholding the constraints over the considered interval. The discrete equations of motion thereby follow as

$$\Delta\mathbf{q} \;=\; \frac{\partial H_*}{\partial\mathbf{p}^T} \;=\; h\,\mathbf{G}(\bar{\mathbf{q}})^T\mathbb{J}^{-1}\overline{\mathbf{G}(\mathbf{q})\,\mathbf{p}}\,, \tag{23}$$

$$\Delta\mathbf{p} \;=\; -\frac{\partial H_*}{\partial\mathbf{q}^T} \;=\; -\,h\,\mathbf{G}(\bar{\mathbf{p}})^T\mathbb{J}_0^{-1}\overline{\mathbf{G}(\mathbf{p})\,\mathbf{q}} \,-\, h\left[\frac{\partial V_*}{\partial\mathbf{q}^T} \,+\, \left(\frac{\partial\boldsymbol{\Phi}_*}{\partial\mathbf{q}}\right)^T\boldsymbol{\lambda} \,-\, \mathbf{C}(\bar{\mathbf{q}})^T\gamma\right], \tag{24}$$

along with incremental form of constraint condition

$$\Delta\boldsymbol{\Phi} \;=\; \frac{\partial\boldsymbol{\Phi}_*}{\partial\mathbf{q}^T}\Delta\mathbf{q} \;=\; \mathbf{0}\,. \tag{25}$$

The equations (23), (24) and (25) constitute the discrete equivalent to the continuous equations (15), (16) and (17), and satisfy conservation of energy by construction when derived via the finite increment of the Hamiltonian.

Similar to the continuous case, the Lagrange multipliers γ associated with the internal constraints in the discrete dynamic equation (24) can be eliminated via the incremental form of (3), yielding

$$\mathbf{C}(\bar{\mathbf{p}})\,\Delta\mathbf{q} \,+\, \mathbf{C}(\bar{\mathbf{q}})\,\Delta\mathbf{p} \,=\, \mathbf{0}\,. \tag{26}$$

Substitution of the increments of $\mathbf{q}$ and $\mathbf{p}$ from (23) and (24) then leads to an explicit equation for the Lagrange multipliers γ, which can be used to eliminate γ in (24). Hereby the dynamic equation takes the form

$$\begin{aligned}\Delta\mathbf{p} \,=\, &-\,h\,\mathbf{G}(\bar{\mathbf{p}})^T\mathbb{J}_0^{-1}\overline{\mathbf{G}(\mathbf{p})\,\mathbf{q}} \,+\, h\,\mathbf{C}(\bar{\mathbf{q}})^T\gamma_0 \\ &-\,h\left(\mathbf{I} \,-\, \mathbf{C}(\bar{\mathbf{q}})^T\left[\mathbf{C}(\bar{\mathbf{q}})\,\mathbf{C}(\bar{\mathbf{q}})^T\right]^{-1}\mathbf{C}(\bar{\mathbf{q}})\right)\left[\frac{\partial V_*}{\partial\mathbf{q}^T} \,+\, \left(\frac{\partial\boldsymbol{\Phi}_*}{\partial\mathbf{q}}\right)^T\boldsymbol{\lambda}\right],\end{aligned} \tag{27}$$

where the term

$$\gamma_0 \,=\, \left[\mathbf{C}(\bar{\mathbf{q}})\,\mathbf{C}(\bar{\mathbf{q}})^T\right]^{-1}\left[\mathbf{C}(\bar{\mathbf{q}})\mathbf{G}(\bar{\mathbf{p}})^T \,+\, \mathbf{C}(\bar{\mathbf{p}})\mathbf{G}(\bar{\mathbf{q}})^T\right]\mathbb{J}^{-1}\overline{\mathbf{G}(\mathbf{p})\,\mathbf{q}}\,. \tag{28}$$

follows from the direct discretization and is needed for ensuring the conservative properties.

Table 1. Conservative time integration algorithm for multibody system.

1)	Initial conditions: $\mathbf{u}_0^T = [\mathbf{q}^T, \mathbf{p}^T, \mathbf{0}^T]_0$
2)	Prediction step: $\mathbf{u} = \mathbf{u}_n$,
3)	Residual calculation: $\mathbf{r} = \mathbf{r}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda})$ from (30).
4)	Update incremental rotation parameters: $\delta\mathbf{u} = -\mathbf{K}_*^{-1}\,\mathbf{r}$, with $\mathbf{K}$ from (33). $\mathbf{u} = \mathbf{u} + \delta\mathbf{u}$, If $\|\mathbf{r}\| > \varepsilon_{\rm r}$ repeat from 3).
5)	Return to 2) for new time step, or stop.

5 Multibody systems

The above derived equations of motion for a single rigid body can easily be generalized to account for multiple bodies connected by kinematic joints. Consider a system consisting of n bodies linked together by m external constraints via Lagrange multipliers. For each body I the 12 generalized coordinates are collected in the vector $\mathbf{q}^I$, while the conjugate momentum components are stored in the vector $\mathbf{p}^I$, $I = 1\ldots, n$. The phase-space vector for each body is then introduced as $\mathbf{u}^I = [(\mathbf{q}^I)^T, (\mathbf{p}^I)^T]^T$, while m Lagrange multipliers associated with external constraints are collected in vector $\boldsymbol{\lambda} = [\lambda_1, \ldots, \lambda_m]^T$.

For each body I, the equations of motion are given by (23) and (28). The kinematic equation (23) only depend on the variables $\mathbf{q}^I$ and $\mathbf{p}^I$, while the coupling between the motion of different bodies occurs in the dynamic equation (28) trough constraint relations of the form (25). It is therefore convenient to arrange all the independent variables of the multibody system in the system vector

$$\mathbf{u}^T = \left[\; (\mathbf{u}^1)^T, \quad (\mathbf{u}^2)^T, \quad \ldots \quad (\mathbf{u}^n)^T, \quad \boldsymbol{\lambda}^T \;\right]. \tag{29}$$

The full system is solved by means of Newton-Raphson iterations, where the elements of the residual vector $\mathbf{r}^I$ are defined as the difference between the left and the righthand side of (23), (28) and (25). These are conveniently organized in the system residual vector $\mathbf{r}$, given by

$$\mathbf{r}^T = \left[\; (\mathbf{r}^1)^T, \quad (\mathbf{r}^2)^T, \quad \ldots \quad (\mathbf{r}^n)^T, \quad \mathbf{r}_\lambda^T \;\right], \tag{30}$$

where the last element $\mathbf{r}_\lambda$ holds the residuals associated with the m constraint equations of the form (25). The residual is reduced iteratively to zero via the linearized increment $\delta\mathbf{u}$, which is obtained by solving the equation

$$\mathbf{K}_*\delta\mathbf{u} = -\mathbf{r}\,. \tag{31}$$

The system tangential matrix can be obtained by partial differentiation as

$$\mathbf{K}_* = \begin{bmatrix} \mathbf{K}_{ij} & \left(\partial\boldsymbol{\Phi}/\partial\mathbf{u}^I\right)^T \\ \partial\boldsymbol{\Phi}/\partial\mathbf{u}^I & \mathbf{0} \end{bmatrix}, \tag{32}$$

where the matrix $\mathbf{K}_{ij}$ is a block-diagonal form of the contributions from each of the bodies in the system given by

$$\mathbf{K}_{ij} = \sum_I \frac{\partial\mathbf{r}_i^I}{\partial\mathbf{u}_j^I}\,. \tag{33}$$

It is noted that a symmetric structure in (32) has been obtained by embedding the time step h in the system vector (29) on $\boldsymbol{\lambda}$.

The implementation of the algorithm is illustrated in pseudo-code format in Table 1 with a convergence criterion specified in terms of the parameter ε_r. In particular, the Lagrange multipliers are constant within each interval and may be discontinuous over the intervals, hence the initial value $\boldsymbol{\lambda}_0 = \mathbf{0}$ included in the initial conditions is merely a formal construct to establish the full vector $\mathbf{u}_0$ needed for initiating the iteration process.

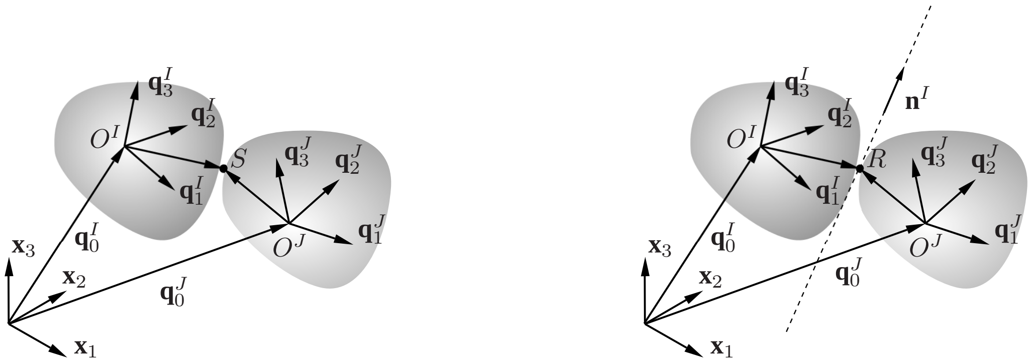

Figure 1. Lower-pair joints: (a) Spherical joint, (b) Revolute joint.

5.1 Kinematic constraints

In the present context only lower-pair kinematic joints expressed by holonomic constraints of the form (17) are considered. Often these are used to describe a distance or an angle by relations, which are at most quadratic in the generalized displacements, hence explicit expressions for the finite derivative with respect to $\mathbf{q}$ can be obtained. In particular two commonly used joints are presented: Spherical joints and revolute joints.

A spherical joint between body I and body J prevents relative motion of the bodies with respect to a common point S, but allows the bodies to rotate freely relative to each other. This is illustrated in Fig. 1(a), and can be expressed in terms of the three algebraic equations

$$\mathbf{\Phi}^{(S)}(\mathbf{q}) \;=\; \mathbf{q}_0^J + x_j^{S,J}\mathbf{q}_j^J \;-\; (\mathbf{q}_0^I + x_j^{S,I}\mathbf{q}_j^I) \;=\; \mathbf{0}\,, \tag{34}$$

where $x_j^{S,I}$ and $x_j^{S,J}$ denote the local coordinates of the point S in the bodies I and J, respectively. The corresponding constraint Jacobian follow from differentiation as the 3×24 constraint matrix

$$\frac{\partial \mathbf{\Phi}^{(S)}}{\partial \mathbf{q}} \;=\; \begin{bmatrix} -\mathbf{I} & -x_1^{S,I}\mathbf{I} & -x_2^{S,I}\mathbf{I} & -x_1^{S,I}\mathbf{I} & \mathbf{I} & x_1^{S,J}\mathbf{I} & x_2^{S,J}\mathbf{I} & x_1^{S,J}\mathbf{I} \end{bmatrix}. \tag{35}$$

This is constant with respect to $\mathbf{q}$, hence (35) constitute an explicit expression for the finite derivative $\partial\mathbf{\Phi}_*/\partial\mathbf{q}$ needed for ensuring the conservative properties of the discretized equations of motion.

A revolute joint between bodies I and J as illustrated in Fig. 1(b) only permits relative rotation about a fixed axis, hence the three constraints imposing equal position at a global point R equivalent to (34) are supplemented by two orthogonality conditions restraining relative rotation of the bodies about two orthogonal axis. This is conveniently described by means of an unit vector $\mathbf{n}$ fixed in body I with constant components n_j with respect to the base vectors $\mathbf{q}^I$, as

$$\mathbf{n} \;=\; n_j\,\mathbf{q}_j^I\,. \tag{36}$$

The five constraint equations can then be expressed in the form

$$\mathbf{\Phi}^{(R)}(\mathbf{q}) \;=\; \begin{bmatrix} \mathbf{q}_0^J + x_j^{R,J}\mathbf{q}_j^J \;-\; (\mathbf{q}_0^I + x_j^{R,I}\mathbf{q}_j^I) \\ (\mathbf{n}^I)^T\mathbf{q}_2^J \\ (\mathbf{n}^I)^T\mathbf{q}_3^J \end{bmatrix} \;=\; \mathbf{0}\,, \tag{37}$$

with the 5×24 gradient matrix, given by

$$\frac{\partial \mathbf{\Phi}^{(R)}}{\partial \mathbf{q}} \;=\; \begin{bmatrix} -\mathbf{I} & -x_1^{R,I}\mathbf{I} & -x_2^{R,I}\mathbf{I} & -x_1^{R,I}\mathbf{I} & \mathbf{I} & x_1^{R,J}\mathbf{I} & x_2^{R,J}\mathbf{I} & x_1^{R,J}\mathbf{I} \\ \mathbf{0}^T & n_1(\mathbf{q}_2^J)^T & n_2(\mathbf{q}_2^J)^T & n_3(\mathbf{q}_2^J)^T & \mathbf{0}^T & \mathbf{0}^T & (\mathbf{n}^I)^T & \mathbf{0}^T \\ \mathbf{0}^T & n_1(\mathbf{q}_3^J)^T & n_2(\mathbf{q}_3^J)^T & n_3(\mathbf{q}_3^J)^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & (\mathbf{n}^I)^T \end{bmatrix}. \tag{38}$$

It is seen that contrary to (35), the gradient matrix for a revolute joint depends on the current configuration.

6 Numerical examples

The accuracy and conservative properties of the present algorithm for multibody systems are illustrated in terms of a hanging chain represented by 4 rigid bodies connected by revolute joints and spherical joints, respectively.

6.1 Hanging chain with revolute joints

First the case where the bodies are linked together by revolute joins is considered. Each body is represented as a box with side lengths $[1, 0.5, 3]$ and mass $M = 12$. The principal moment of inertia tensor with respect to the center of mass is then given by $\boldsymbol{J} = \text{diag}[9.25, 10.0, 1.25]$. The motion of the chain is initiated by releasing it from the initial position illustrated in Fig. 2(a) where the bodies 1 and 2 are inclined by an angle $\theta_1 = \pi/4$ with respect to vertical. The bodies 3 and 4 are rotated by $3\pi/4$, thereby forming a right angle with the bodies 1 and 2.

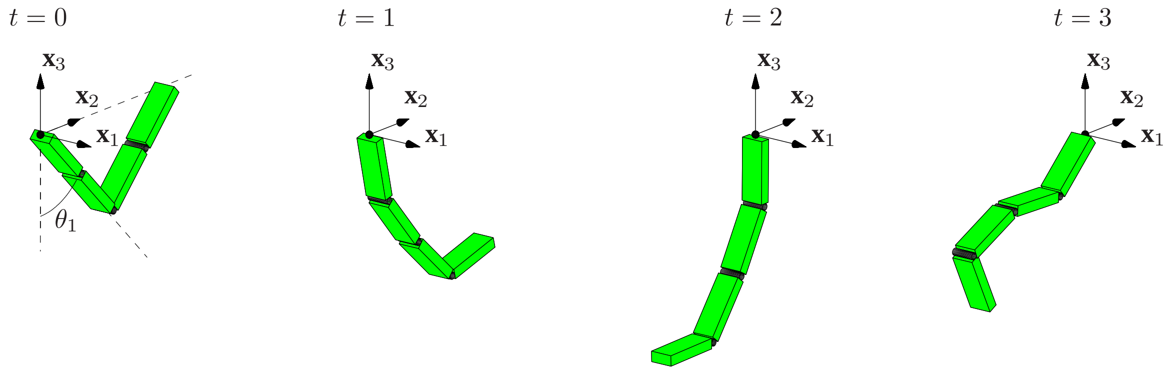

Figure 2. Motion of chain with revolute joints at selected points in time.

The chain is located in a uniform gravitational field with acceleration $g = 9.81$ in the negative x_3-direction acting at the center of mass $\mathbf{q}_0^I$ for each body I. This corresponds to the potential energy

$$V(\mathbf{q}) = \sum_I M^I \mathbf{g}^T \mathbf{q}_0^I , \tag{39}$$

with the gravitational acceleration vector $\mathbf{g}^T = [0, 0, -g]$. The considered constrained system is indeed conservative, and thus the total mechanical energy as well as the 3-component of the angular momentum vector l_3 are conserved quantities. The angular momentum with respect to the origin of the global $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ coordinate system can be evaluated as

$$\mathbf{l} = \sum_I \mathbf{q}_0^I \times M^I \mathbf{v}^I + \mathbf{Q}^I (\mathbf{J}^I \boldsymbol{\Omega}^I) , \tag{40}$$

where the first term accounts for translational motion of the center of mass, while the second term represents the rotational motion.

The external constraint equations associated with the revolute joints can be expressed by (37) with $n_j = [1, 0, 0]^T$. It is important to notice that since the gradient (38) depend on the director components $\mathbf{q}$, its algorithmic form is represented by its finite derivative. The constraint equations (37) are quadratic in $\mathbf{q}$, hence their incremental form can be expressed as twice the product of the mean of one factor plus the increment of the other as

$$\Delta \boldsymbol{\Phi}^{(R)}(\mathbf{q}) = \Delta \mathbf{q}^T \frac{\partial \boldsymbol{\Phi}_*}{\partial \mathbf{q}^T} = \Delta \mathbf{q}^T \frac{\partial \boldsymbol{\Phi}^{(R)}(\bar{\mathbf{q}})}{\partial \mathbf{q}^T} , \tag{41}$$

whereby the algorithmic form of the constraints gradient follows as

$$\frac{\partial \boldsymbol{\Phi}_*}{\partial \mathbf{q}} = \frac{\partial \boldsymbol{\Phi}^{(R)}(\bar{\mathbf{q}})}{\partial \mathbf{q}} . \tag{42}$$

In the present rigid body formulation each body is represented by 12 redundant coordinates along with 6 internal constraints of the type (3). However, these are included implicitly when the modified dynamic equation (28) is used. Furthermore, each revolute joint yields a set of 5 external constraint equations of the form (37). Since these are imposed explicitly via Lagrange multipliers, the constrained mechanical system under consideration yields $12n + m = 68$ unknowns.

The motion of the chain after initial release is illustrated in Fig. 2(a)-(d) at consecutive instances in time. The development of the total mechanical energy is illustrated in Fig. 3(a) for a time step of $h = 0.01$. Algorithmic conservation is obtained within an accuracy of 10^{-12}, which is well below the convergence tolerance of $\varepsilon_r = 10^{-8}$. Furthermore, the components of the angular momentum vector $\mathbf{l}$ are shown in Fig. 3(b) with $\mathbf{l}_1$ as the only non-zero component as motion is limited to the $\mathbf{x}_2\mathbf{x}_3$-plane.

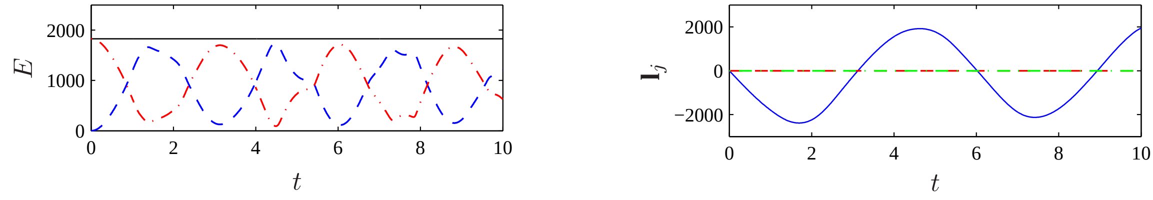

Figure 3. Chain with revolute joints: (a) Total mechanical energy, E (–), T (- -), V (-·-), (b) Angular momentum. $\mathbf{l}_1$ (–), $\mathbf{l}_2$ (- -), $\mathbf{l}_3$ (-·-).

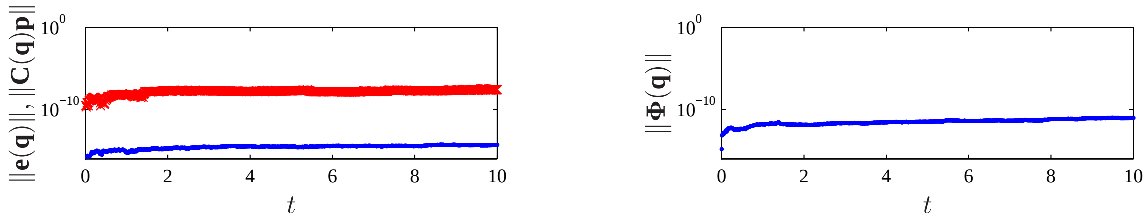

Figure 4. Satisfaction of constraints: (a) Internal constraints, $\mathbf{e}(\mathbf{q})$ (•), $\mathbf{C}(\mathbf{q})\mathbf{p}$ (×), (b) External constraints.

The algorithmic satisfaction of the internal constraints, i.e. the zero strain constraints (3) and the displacement-momentum orthogonality relation (18) is illustrated in Fig. 4(a). Similarly the violation of the external constraints associated with the spherical joints, (34) is shown in Fig. 4(b), and it is seen that the errors in all three cases are below the iteration tolerance.

6.2 Hanging chain with spherical joints

In this example the hanging chain illustrated in Fig. 5(a) is considered. The properties of the chain are equivalent to the ones described above. However, now the revolute joints between the rigid bodies are replaced by spherical joints allowing free relative rotation between adjacent bodies at their common points. Theses are expressed in the form (34), hence problem has $12n + m = 60$ unknowns. The finite derivative $\partial \boldsymbol{\Phi}_* / \partial \mathbf{q}$ is given directly by (35).

The motion of the chain is initiated from an initial state similar to the previous example as illustrated in Fig. 5(a). However, the chain is now rotated an angle $\theta_2 = \pi/4$ about the $\mathbf{x}_2$ axis, thereby introducing out-of-plane motion.

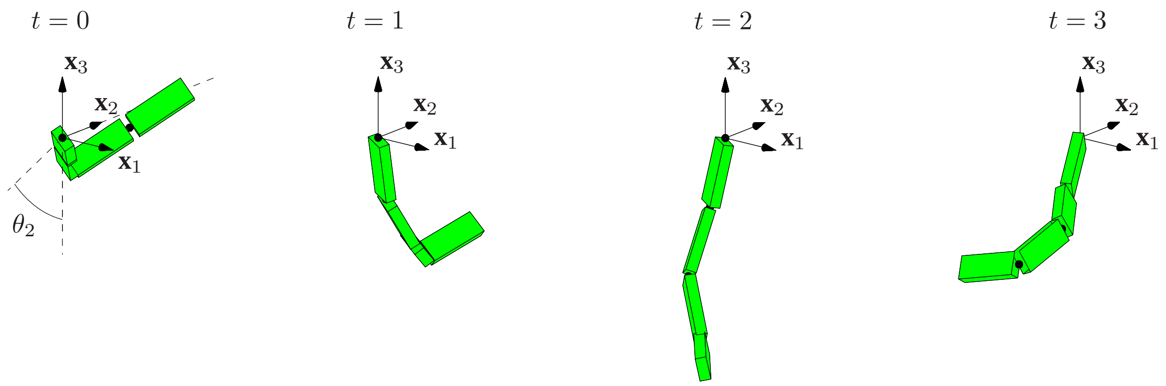

Figure 5. Motion of chain with spherical joints at selected points in time.

The motion at selected points in time is illustrated in Fig. 5, while the development of energy an angular momentum are presented in Fig. 6(a) and 6(b) for a time step of $h = 0.1$. The total mechanical energy and the l_3-component of the angular momentum are conserved within an accuracy of 10^{-12} and 10^{-10}, respectively, for an iteration tolerance of $\varepsilon_r = 10^{-8}$. Similarly internal as well as external constraints are satisfied to well below the iteration tolerance as shown in Fig. 7(a) and (b).

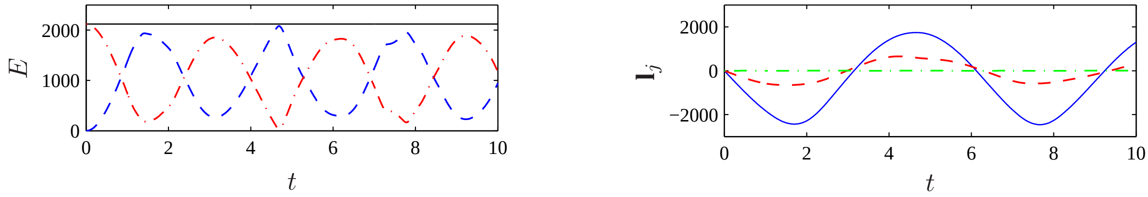

Figure 6. Chain with spherical joints: (a) Total mechanical energy, E (–), T (- -), V (-·-), (b) Angular momentum. $\mathbf{l}_1$ (–), $\mathbf{l}_2$ (- -), $\mathbf{l}_3$ (-·-).

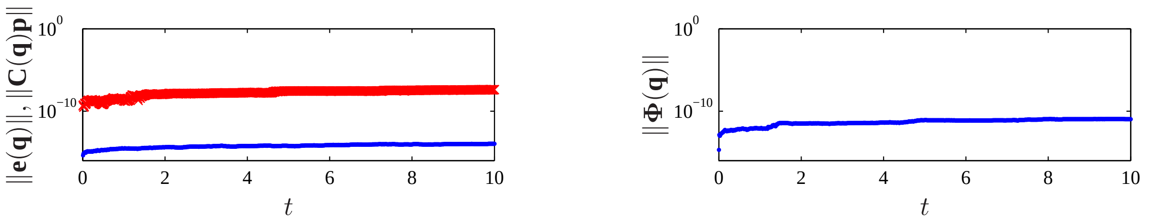

Figure 7. Satisfaction of constraints: (a) Internal constraints, $\mathbf{e}(\mathbf{q})$ (•), $\mathbf{C}(\mathbf{q})\mathbf{p}$ (×), (b) External constraints.

7 Conclusions

A momentum and energy conserving time integration algorithm has been presented for constrained mechanical systems consisting of multiple rigid bodies. The independent variables are the three translation components and a convected set of 3×3 orthonormal base vectors components for each rigid body. The equations of motion are derived from Hamilton's equations where internal constraints enforcing orthonormality of the base vectors and external constraints associated with the presence of kinematic joints are included initially via Lagrange multipliers. Subsequently the Lagrange multipliers associated with the internal constraints are eliminated by a set of displacement-momentum orthogonality relations, leaving only a projection on the potential gradient and external constraint gradient. A consistent discretization satisfying conservation of energy and momentum is identified by equating the finite increment of the Hamiltonian to zero. In particular, constraints are enforced in incremental form, whereby the corresponding Lagrange multipliers can be represented as constant effective mean values associated with the interval. This approach is illustrated for systems including both internal and external constraints.

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